NASCRE-5 Oral Presentation Program

Sunday, February 16: Workshops (11:30-16:30) &
Welcome Reception (18:00-19:30) Monarch Room (Level 24)

Day 1: Monday, February 17				
	Galleria I & II			
8:00-8:15 AM	Opening Remarks (Praveen Bollini)			
8:15-9:15 AM	Plenary: Developing Strategies for Polymer Redesign and Recycling Using Reaction Pathway Analysis ***Linda Broadbelt*** *(Northwestern University)*			
9:15-9:30 AM	Refreshment Break			
9:30-10:30 AM	Plenary: Amundson Award Presentation (ExxonMobil) and Lecture A Personal Journey to Reaction Engineering: From Multiscale Modeling to Sustainable Processes ***Dion Vlachos*** *(University of Delaware)*			
10:30-10:45 AM	Break			
	Galleria I & II	Galleria III	Tanglewood/Bellaire	Post Oak
	Polymer Upcycling Chairs: Alan Stottlemeyer (Dow), Michele Sarazen (Princeton)	**Fundamentals of CRE** Chairs: Hilal Ezgi Toraman (Penn State), Gregory Patience (Polytechnique Montreal)	**Reaction Engineering for the Energy Transition: 1** Chairs: Pavel Kots (NYU), Daniel Trahan (Dow)	**Novel Reactors and Process Intensification: 1** Chairs: Chris Paolucci (UVa), Dongxia Liu (U. Delaware)
10:45-11:05 AM	Revealing the Role of Mass Transfer–Chemical Kinetics Coupling in Neat and Catalytic High-Density Polyethylene Pyrolysis; *M.* ***Doga Tekbas*** *(U Mass. Lowell)*	Keynote: Harnessing Coupled Reaction-Transport Phenomena to Develop Stable and Selective Catalysts for Olefin Oligomerization to Transportation Fuels; ***Rajamani Gounder*** *(Purdue University)*	Modeling of a Heat-Integrated Biomass Downdraft Gasifier with Construction and Demolition Waste as Feedstock; ***Kim McAuley*** *(Queens University)*	Microfluidic Laser-Induced Nucleation of Iron (II, III) Oxide Nanoparticle-Doped Supersaturated Aqueous KCl solutions; ***Kelechi Ndukwe-Ajala*** *(NYU)*
11:05-11:25 AM	Understanding Reaction Environments in Mechanocatalytic Processes; ***Carsten Sievers*** *(Georgia Tech)*	Length Effects of PRCFD-Derived Fixed Bed Radial Heat Transfer; ***Anthony Dixon*** *(WPI)*	Radio Frequency Heating of Catalytic Propane Dehydrogenation: Finite Element Approach, Techno-Economic, and Environmental Assessment. ***Ankush Rout*** *(Texas A&M University)*	Novel modular, layered rector for continuous, scalable, efficient hydrogenation; ***Lorenzo Milani*** *(Zaiput Flow Technologies)*
11:25-11:45 AM	H_2-Free Conversion of Condensation Polymers with Organic H2 Carriers - Kinetic Coupling of Hydrogenolysis and Dehydrogenation Pathways; ***Manish Shetty*** *(Texas A&M University)*	Mechanistic and Kinetic Role of Pd in the Co-Production of Ethylene and Acetic Acid from Ethane over Pd-MoV Oxides; ***Joseph Lane*** *(University of Houston)*	Mechanistic Insights into Sustainable Chemical Processes: Oxygen Electrocatalysis and Fischer-Tropsch Synthesis; ***Kasun Gunasooriya*** *(University of Oklahoma)*	Mechanistic Aspects of Selective Hydrogen Combustion (SHC) over NA_2WO_4/SIO_2 Catalysts; ***Elijah Kipp*** *(University of Minnesota)*
11:45-1:15 PM	Lunch on own			
	Galleria I & II			
1:15-2:15 PM	Panel Discussion: 'Academia-Government-Industry: Advancing Reaction Engineering at the Interfaces Facilitator: **Nick Thornburg** (NREL) Panelists: **Jean Tom** (Princeton University), **Fabio Ribeiro** (Purdue University), **Simon Bare** (SLAC), **Triantafillos J. Mountziaris** (University of Houston)			
2:15-2:30 PM	Break			
	Pioneers in CRE: 1 Chairs: Ryan Hartman (NYU), Moiz Diwan (AbbVie)	**Fundamentals of CRE** Chairs: Nitish Mittal (ExxonMobil), Udit Gupta (Siemens)	**Reaction Engineering for the Energy Transition: 2** Chairs: Hsu Chiang (Oxy), Joseph Dewilde (Dow)	**Novel Reactors and Process Intensification: 2** Chairs: Rajamani Gounder (Purdue), Eric Sacia (AbbVie)
2:30-2:50 PM	Elucidating complex interactions in non-thermal plasma-assisted reactions on (supported) porous catalysts ***Michele Sarazen*** *(Princeton)*	Quantifying Reaction-Diffusion Rates of Nonoxidative Coupling of Methane per Active Edge Sites of Two-Dimensional Pt Nanolayer Catalysts; ***Tobias Misicko*** *(Louisiana Tech)*	Decarbonization of Hydrogen Supply Chain via Electrification: Methane Reforming and Ammonia Decomposition ***Ram Ratnakar*** *(Shell)*	Forced Dynamic Operation of Propylene Selective Oxidation on Bismuth-Molybdate Structured Catalysts: Experiments and Modeling; ***Mohammad Moniruzzaman*** *(University of Houston)*
2:50-3:10 PM	Fast-Cat: A Self-Driving Catalysis Lab for Autonomous Reaction Pareto Front Mapping ***Milad Abolhasani*** *(North Carolina State University)*	A new method for the simulation of catalyst deactivation in fluidized bed reactors; ***Andrea Pappagallo*** *(Paul Scherrer Institut)*	Catalytic and Inhibitory Effects Induced by Noncovalent Interactions between Cellulose and Lignin During Fast Pyrolysis; ***His-Wu Wong*** *(U Mass Lowell)*	Selective Chemical Looping Combustion of Acetylene in Ethylene-Rich Streams; ***Matthew Jacob*** *(University of Minnesota)*
3:10-3:30 PM	Effect of Blending Hydrogen with Natural Gas on Selective Catalytic Reduction of NOx for Stationary Power Applications ***Bihter Padak*** *(UC Irvine)*	Redefining Bi-reforming of Methane at a Molecular Level Through Specific Metal-Support Interactions; ***Meghana Sucharita Idamakanti*** *(University of Houston)*	Highly Efficient and Stable Iron Molybdate Electrocatalyst towards Oxygen Evolution Reaction under Alkaline Conditions; ***FNU Vidhi*** *(University of Houston)*	CO_2 absorption kinetics measurements: conversion of a stirred tank to a Lewis cell; ***Jonathan Sheavly*** *(Dow)*

3:30-3:50 PM	Refreshment Break			
	Pioneers in CRE: 2 Chairs: Ryan Hartman (NYU), Moiz Diwan (AbbVie)	**Fundamentals of CRE** Nitish Mittal (ExxonMobil), Udit Gupta (Siemens)	**Reaction Engineering for the Energy Transition: 3** Chairs: Hsu Chiang (Oxy), Joseph Dewilde (Dow)	**Novel Reactors and Process Intensification: 3** Chairs: Fateme Rezaei (U. Miami), Onkar Manjrekar (Abbvie)
3:50-4:10 PM	Electrocatalytic Synthesis and Utilization of Nitrates for Resilient Nitrogen Circular Economy ***Meenesh Singh*** *(University of Illinois Chicago)*	From Pulses to Pellets to Packed Beds: Understanding $CrOx/Al_2O_3$ Catalyst Deactivation during Propane Dehydrogenation via Transient Kinetic Analysis and Multiscale Modeling; ***Nicholas Thornburg*** *(NREL)*	Experimental Analysis of a Sabatier reactor for Renewable Natural Gas Generation from Biogas: Ignition, Parameter Sensitivity Analysis, and Stability; ***David Simakov*** *(Univ. Waterloo)*	Applications of Countercurrent Multiphase Reactors for Maximizing Performance ***James R. Lattner*** *(Exxon, retired)*
4:10-4:30 PM	Catalytic consequences of plastic additives on bifunctional reactions of alkanes ***Gina Noh*** *(Penn State)*	Polymer Distribution Models for Polyether Polyols; ***Arjun Raghuraman*** *(Dow)*	Electrification of Steam Methane Reforming by Joule Heating of Nickel-Coated High-Resistance Wires; ***Elmer Ledesma*** *(University of Houston)*	Overcoming the Selectivity-Conversion Tradeoff during Forced Dynamic Operation of Ethane Oxidative Dehydrogenation; ***Austin Morales*** *(University of Houston)*
4:30-4:50 PM	Tackling Climate Change with Chemical Reaction Engineering: Sustainable Aviation Fuel Production Challenges and Solutions ***Kathryn Bjorkman*** *(LanzaJet)*	From Apparent Kinetics to Microkinetics: Leveraging Power duLaw Models for Reaction Mechanism Identification; ***Fernando Vega-Ramon*** *(Univ. of Manchester)*	Bench-Scale Multi-Tubular Membrane Contactor Reactor for Fuel Production; ***Mohammad Bazmi*** *(USC)*	In-situ characterization of Ni-BaH_2 catalyst for low temperature ammonia production through chemical looping; ***Antoine Dechany*** *(UC Louvain)*

Dinner on own

Day 2: Tuesday, February 18

	Galleria I & II			
8:00-8:15 AM	Opening Remarks (Moiz Diwan)			
8:15-9:15 AM	Plenary: Current Trends and Opportunities for Reaction Engineering to Impact the Pharmaceutical R&D Pipeline ***Shailendra Bordawekar*** *(AbbVie)*			
9:15-9:30 AM	Refreshment Break			
9:30-10:30 AM	Plenary: Aris Award Presentation (ISCRE) and Lecture The Many Lives of Active Oxygens in the Energy Transition ***Praveen Bollini*** *(University of Houston)*			
10:30-10:45 AM	Break			
	Galleria I & II	Galleria III	Tanglewood/Bellaire	Post Oak
	Computational Chemistry and Catalysis, Data Science, ML: 1 Milad Abolhasani (NCSU), Gaurav Giri (UVa)	**Automation/Digitization in Reaction Engineering: 1** Chairs: Jake Gold (Dow), Meenesh Singh (UIC)	**Reaction Engineering for the Energy Transition: 4** Chairs: Hsi-Wu Wong (UMass Lowell), Kim McAuley (Queens University)	**Novel Reactors and Process Intensification: 4** Chairs: Fateme Rezaei (U. Miami), Onkar Manjrekar (Abbvie)
10:45-11:05 AM	Using Molecular Modeling and Machine Learning to Address Stability Challenges for Zeolite Catalysts ***Chris Paolucci*** *(University of Virginia)*	Hybrid Modeling for the Dynamic Simulation of Water Gas Shift and Methanol Synthesis Reactions Network; ***Fernando Vega-Ramon*** *(University of Manchester)*	Thermodynamic Analysis Based Programmed Heating Strategies to Limit Carbon Depositions in Electrified Modular Methane Reformer Reactors; ***Collins Don-Pedro*** *(University of Houston)*	Ignition-Extinction Analysis of Oxidative Dehydrogenation of Ethane over M1 Catalyst in a Monolith Reactor; ***Dhagash M. Pandit*** *(University of Houston)*
11:05-11:25 AM	Application of surrogate modelling to accelerate design space exploration for catalytic reactor systems; ***Udit Gupta*** *(Siemens)*	Advantages of AI-based models over mechanistic models in the dynamic optimization of fixed- and fluidized-bed reactors; ***Mauro Andrea Pappagallo*** *(Paul Scherrer Institut)*	Dynamic Optimization of Electrified Ethane Cracking for Cost-Effective Ethylene Production with Low CO_2 Emissions; ***Alexandre Cattry*** *(NYU)*	Methane Partial Oxidation (MPO) under Periodic Reaction Conditions on Pt/Al_2O_3; ***William Epling*** *(University of Virginia)*
11:25-11:45 AM	Advantages in the use of AI-based regressions for the kinetic modelling of industrial catalysts; **Emanuele Moioli** *(Politecnico di Milano)*	Investigating a Novel Flash Thermal Racemisation Reaction Operated Under Transient Flow Regimes through Kinetic Modelling; ***Harry Kay*** *(University of Manchester)*	Towards the complete mineralization of PFOA with a pilot-scale UV-light, boron-nitride—based recirculating reactor unit; ***Juan Donoso*** *(Rice University)*	Ignition Threshold of Argon Diluted Methane in Atmospheric Plasma-Liquid Multiphase Microreactor; ***Sudip Das*** *(NYU)*
11:45-1:15 PM	Lunch on own			

	Galleria I & II			
1:15-2:15 PM	Panel Discussion: Vision 2050: Reaction Engineering Roadmap Facilitator: **Ryan Hartman** (NYU) Panelists: **Dan Hickman** (Dow), **Kim McAuley** (Queens University), **Michael Harold** (University of Houston)			
2:15-2:30 PM	Break			
	In Honor of the Amundson Awardee: 1 Chairs: Ashish Mhadeshwar (ExxonMobil), Jeffrey Rimer (University of Houston)	**Automation/Digitization in Reaction Engineering: 2** Chairs: Kevin Modica (Dow), Ram Ratnakar (Shell)	**Reaction Engineering for the Energy Transition: 5** Chairs Jeremy Bedard (Oxy), Nick Thornburg (NREL)	**Novel Reactors and Process Intensification: 5** Chairs: Saurabh Bhandari (Dow), Jiakang Chen (BASF)
2:30-2:50 PM	Reaction Engineering: The ISCRE Board's 2050 Perspective ***Dan Hickman*** *(Dow)*	Transforming Reaction Engineering Through Automation and Digitization; ***Jason E. Hein*** *(University of British Columbia)*	1071: Microkinetic Modeling of Oxidative Coupling of Methane: Can Electrochemistry Break the Scaling Relationship?; ***Julian Ufert*** *(MIT)*	Forced Dynamic Operation of Propylene Selective Oxidation to Acrolein in Catalytic Foam Reactor: Reactor Model Development ***Kai Wu*** *(University of Houston)*
2:50-3:10 PM	Propane Dehydrogenation in Electrifiable Carbon Membrane Reactor ***Dongxia Liu*** *(U. Delaware)*	Application of Dynamic Reaction Screening and Development of a 2-D Reactor Model for Accurate Kinetic Analysis in Tubular Reactors; ***Daniel Trahan*** *(Dow)*	*(University of Houston)* Optimization of temperature profiles in CO_2 methanation reactors by an appropriate selection of catalyst and dilution agent; **Emanuele Moioli** *(Politecnico di Milano)*	Can methanol synthesis be enhanced at low pressure with continuous operation?; ***Chiara Berretta*** *(Paul Scherrer Institut)*
3:10-3:30 PM	Multiple Rate States in Precious Metal Catalyzed Oxidation Reactions: Kinetic Requirements, Multiplicity Features and Rate Determining Steps ***Michael P. Harold*** *(University of Houston)*	Model-Based Fault Diagnosis for Closed-loop Feedback controlled Safety-Critical Chemical Reactors: An Experimental Study; ***Pu Du*** *(Texas A&M University)*	Isopotential Titration of Ammonia Electron Transfer on Metal Catalysts; ***Jesse Canavan*** *(Univ. of Minnesota)*	Experimental and modeling of reactive distillation applied for an immobilized enzymatic reaction coated on structured internals; ***Nicolas Chaussard*** *(Université Lyon)*
3:30-3:50 PM	Refreshment Break			
	In Honor of the Amundson Awardee: 2 Chairs: Ashish Mhadeshwar (ExxonMobil), Jeffrey Rimer (University of Houston)	**Automation/Digitization in Reaction Engineering: 3** Chairs: Kevin Modica (Dow), Ram Ratnakar (Shell)	**Reaction Engineering for Materials Synthesis** Jeremy Bedard (Oxy), Nick Thornburg (NREL)	**Computational Chemistry and Catalysis, Data Science, ML** Chairs: Saurabh Bhandari (Dow), Jiakang Chen (BASF)
3:50-4:10 PM	Joule heated structured reactors: combining electrification with process intensification ***Enrico Tronconi*** *(Politecnico di Milano)*	Digital Twin Concept For Hydrogen Production From Biogas; ***Razieh Etezadi*** *(USC)*	Mechanistic Insights into Metal-Organic Framework Formation from In-Situ X-Ray Scattering Data ***Gaurav Giri*** *(University of Virginia)*	Computational Insights into the Behavior of H_2 and CO_2 on Cu and ZnO Surfaces for Methanol Synthesis; ***Haseen Siddiqui (IIT Mumbai)***
4:10-4:30 PM	Advancing Product Analysis and Polymer Recycling Strategies with Two-Dimensional Gas Chromatography (GC×GC) ***Hilal Ezgi Toraman*** *(Penn State)*	CatTestHub: A Benchmarking Database of Experimental Heterogeneous Catalysis and Insights for Methanol Decomposition; ***Atharva Burte*** *(University of Houston)*	A Novel Plasma Enhanced Chemical Vapor Deposition (PECVD) Reactor System for Fabrication of SiC-Type Ceramic Films and Membranes; ***Farnaz Tabarkhoon*** *(USC)*	First principles insights into effect of charge condensation on water gas shift reaction mechanism; ***Venkata Rohit Punyapu*** *(Ohio State University)*
4:30-4:50 PM	Intensification of polyolefin plastic waste hydroconversion in small alkane solvents ***Pavel Kots*** *(NYU)*	From Laboratory to Pilot: Digital Design Case Study for Cost Effective Catalytic Reactor Scale Up; ***Shahin Goodarznia*** *(Nova Chemicals)*	Synthesis of Brightly Fluorescent ZnSe Quantum Dots using Air-Stable Precursors; ***Ali Rad*** *(University of Houston)*	Machine Learning for Parametric Sensitivity of Chemical Reactors; ***Joaquin Herrero*** *(Louisiana Tech University)*
Tuesday, Feb 18: Conference Banquet (18:00-21:30) Monarch Room (Level 24)				

Day 3: February 19				
	Galleria I & II			
8:00-8:15 AM	Opening Remarks (Ryan Hartman)			
8:15-9:15 AM	Plenary: Towards Electrifying Chemical Manufacturing Using Electrolysis ***Paul Kenis*** *(University of Illinois Urbana-Champaign)*			
9:15-9:30 AM	Refreshment Break			
	Galleria I & II	Galleria III	Tanglewood/Bellaire	Post Oak
	CO_2 Capture and Conversion: 1 Chairs: Gina Noh (Penn State), Sweta Somasi (Corteva)	**Biopharmaceutical Reaction Engineering: 1** Chairs: Bryan Patel (Exxon), Jane Shi (Dow)	**General Reaction Engineering: 1** Chairs: Kathryn Bjorkman (LanzaJet), Sukaran Arora (Dow)	**General Reaction Engineering: 2** Chairs: David Simakov (U. Waterloo), Kasun Gunasooriya (U. Oklahoma)
9:30-9:50 AM	Reactive Carbon Capture: Cooperative and Bifunctional Adsorbent-Catalyst Materials and Process Integration for a New Carbon Economy ***Fateme Rezaei*** *(University of Miami)*	Development of continuous hydrogenation for pharmaceutical intermediate from Laboratory to Pilot plant; ***Onkar Manjrekar*** *(AbbVie)*	Academic-Industry Sabbaticals: An Academic Reaction Engineer's Perspective; ***Ryan Hartman*** *(NYU)*	Relationship Between the Observed Reaction Kinetics of Ethylene to Ethylene Oxide with Complex Chlorination and Process Conditions Effect; ***Jake Gold*** *(Dow)*
9:50-10:10 AM	1019: Barriers to Carbon Dioxide Utilization ***Daniel Hickman*** *(Dow)*	Development of Pharmaceutically-Relevant Phospholigands from Lab to Plant via Multi-Stage Flow Chemistry; ***Eric Sacia*** *(AbbVie)*	Improving Selectivity and Stability of Low Temperature Methane Dry Reforming Catalysts through Active Site and Process Tuning; ***Jonathan Lucas*** *(LSU)*	Impact of Intermediate Transfer Rates, Metal Cation Mobility, and Hydrocarbon Pool Mechanisms on the Rates and Selectivity for Tandem CO2 Hydrogenation to Olefins and Fuels; ***Fatima Mahnaz*** *(Texas A&M)*
10:10-10:30 AM	Reaction Pathways, Intermediates, and Site Requirements for CO_2 Methanation over Ni-Ce Mixed Metal Oxides; ***Suchetana Samanta*** *(University of Houston)*	Development and Demonstration of an Ultra-High Temperature Continuous Racemization Process for Recycle of Undesired Atropisomer Waste; ***Kiersten Campbell*** *(Snapdragon Chemistry)*	Controlling Molecular Architectures in Alkoxysilane Hydrolysis and Condensation: Reactor Design and Process Considerations; ***Zhichen Shi*** *(Dow)*	Kinetic Modeling and Optimization of a Pharmaceutical Process with Uncertain Inputs; ***Kim McAuley*** *(Queens University)*
10:30-10:45 AM	Break			
	CO_2 Capture and Conversion: 2 Chairs: Gina Noh (Penn State), Sweta Somasi (Corteva)	**Biopharmaceutical Reaction Engineering: 2** Chairs: Bryan Patel (Exxon), Jane Shi (Dow)	**General Reaction Engineering: 3** Chairs: Kathryn Bjorkman (LanzaJet), Sukaran Arora (Dow)	**General Reaction Engineering: 4** Chairs: David Simakov (U. Waterloo), Kasun Gunasooriya (U. Oklahoma)
10:45-11:05 AM	Development of Dual-Function Materials for Reactive Capture of CO_2 from Dilute Stream to Produce CO at High Selectivity; ***Anh To*** *(NREL)*	Transport-Kinetic Modeling of a Double N-Debenzylation in the Production of an Active Pharmaceutical Ingredient ***Neda Nazemifard*** *(Takeda)*	Promotional Role of Acid Sites on Aluminosilicate-Supported Catalysts; ***Welman Elias*** *(Rice)*	A Simple Evaluation of Adiabatic Proton Tunneling across the Electrified Double Layer ***Mahsa Askari*** *(Texas Tech)*
11:05-11:25 AM	Enhanced Performance of Cu/ZrO_2 Catalysts in CO_2 Hydrogenation to Methanol; ***Mohd Moiz Khan*** *(NIT Srinagar)*	Automated Discovery of Enzymatic Reaction Kinetics using Symbolic Regression and Model-Based Design of Experiments; ***Harry Kay*** *(University of Manchester)*	Effects of Feedstock on Yields and Char Properties of Bench Scale Acid Hydrolysis and Dehydration (AHDH) Reaction; ***Ehsan Ullah Sardar*** *(University of Maine)*	Proximity Effects for Improving Ethyl Acetate Selectivity in the Dehydrogenative Coupling of Ethanol over supported Cu Catalysts; ***Varad Joshi*** *(University of Houston)*
11:25-11:45 AM	Closing Remarks - Galleria I & II			

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